NERL Research Abstract

EPA's National Exposure Research Laboratory
GPRA Goal 1 - Clean Air
APMs # 233 and # 528

Significant Research Findings

Extension of the EPA Models-3/ Community Multiscale Air Quality Modeling System to Atmospheric Mercury

Purpose

Many areas of the United States currently have public advisories regarding the consumption of mercury-contaminated fish. Atmospheric deposition is the primary source of this contamination in nearly every case. To help identify the air emission sources of mercury, new CMAQ software has been developed to simulate the emission, transport, chemical and physical transformation, and wet and dry deposition of atmospheric mercury. The new pollutant species added to CMAQ for atmospheric mercury are: elemental mercury (Hg^0), mercuric chloride ($HgCl_2$), mercuric oxide gas (HgO(g)), mercuric oxide aerosol (HgO(a)), and a general mercuric aerosol (HgA) resulting from the evaporation of cloud water containing various dissolved mercury compounds.

Research Approach

The CMAQ model with the new mercury science modules (CMAQ-Hg) has been developed from the June 2000 CMAQ public release version. Current understanding of atmospheric mercury indicates that emissions of sulfur dioxide, volatile organic compounds, and carbon-rich particulate aerosols have important effects on chemical and physical transformations of mercury in air and in cloud water. Thus, the CMAQ's "one-atmosphere" approach involving comprehensive multi-pollutant simulation is well suited to the study of atmospheric mercury cycling and the eventual assessment of source-receptor relationships. In addition to the pre-existing CMAQ model chemistry, the CMAQ-Hg model simulates two gas-phase reactions, eight aqueous-phase reactions, and six dissociation equilibria for mercury and mercury compounds. These reactions were all identified in the scientific literature along with their associated rate and equilibrium coefficients. In addition to chemical reactions, a physical adsorption of all divalent mercury compounds to carbon aerosol suspended in cloud water is also simulated. Anthropogenic emissions of mercury for the CMAQ-Hg model are based on an emissions inventory developed at EPA's Office of Air Quality Planning and Standards and chemical/physical emissions speciation assumptions developed at NERL.

Major Findings

A 24-hour simulation of emission, transport, transformation, and wet and dry deposition of mercury, along with all the standard pollutant species of the CMAQ model, was performed for a northeast United States test domain for July 13, 1995. While the spatial coverage of precipitation for this period was rather small, the cloud chemistry of the model was active over a large fraction of the model domain, especially during the afternoon and evening. Most of the simulated dry deposition of mercury for this modeled period is attributable to dry deposition of emissions of $HgCl_2$ gas before they are involved in cloud chemistry and wet deposition. Both the wet and dry deposition patterns show maximum values for the 24-hour simulation period that are reasonable based on general observations in the United States over the past few years. Despite significant measurement uncertainties that remain in the atmospheric chemistry and emissions of mercury, this research version of CMAQ-Hg can be used now along with supporting observational data to help identify the most important uncertainties in the context of current research regarding atmospheric mercury cycling. As the understanding of atmospheric mercury improves, advances can be efficiently incorporated into the modular CMAQ modeling framework.

Research Collaboration and Publications

The research leading to this new version of the CMAQ model benefitted from collaborative work for atmospheric chemistry of mercury with scientists at the University of Michigan under EPA Cooperative Agreement CR827079, and by NERL's participation in a mercury model intercomparison involving modeling researchers from the United States, Germany, Sweden, and Russia.

Bullock, O.R., Jr. Current methods and research strategies for modeling atmospheric mercury. *Fuel Processing Technology* 65/66: 459-471, 2000.

Future Research

Model simulations will be conducted to study the CMAQ model's ability to replicate mercury wet deposition patterns over the United States and also to perform diagnostic studies using intensive surface and aircraft data collected over Florida.

Questions about CMAQ-Hg modeling system may be directed to:
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